

# Ab initio calculation of the Hoyle state and a new look at clustering in nuclei

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**Abstract.** I present an *ab initio* calculation of the spectrum of  $^{12}\text{C}$ , including also the famous Hoyle state. Its structure is discussed and a new interpretation of clustering in nuclear physics is given.

## 1. What is so special about the Hoyle state?

In 1953, Fred Hoyle analyzed the production of heavy elements like  $^{12}\text{C}$  or  $^{16}\text{O}$  in massive stars. He found that by far too few  $^{12}\text{C}$  was formed if the so-called triple-alpha process would proceed via the ground state of the carbon nucleus. Consequently, Hoyle predicted a  $0^+$ -resonance in the vicinity of the  $^4\text{He}$  plus  $^8\text{Be}$  threshold that increases the carbon production by many orders of magnitude [1]. This excited state was firmly established experimentally at Caltech in 1957 [2]. Ever since, the Hoyle state has been an enigma for nuclear structure theory. For example, *ab initio* calculations<sup>1</sup> based on the successful no-core-shell-model utilizing modern nuclear forces between two and three nucleons do very well in the description of the spectra of p-shell nuclei but fail miserably with respect to the Hoyle state (or its analogs), see [3, 4]. On the contrary, alpha cluster models as discussed in this conference by Martin Freer [5] are quite successful in describing the Hoyle state and other similar excited states in  $^{12}\text{C}$  and  $^{16}\text{O}$ , but with little connection to the underlying few-nucleon forces (see also the recent review [6]). In such type of models, the Hoyle state has a spatial extension that is more than 1.5 times larger than the ground state which seems to be consistent with precision data on electromagnetic transitions, see e.g. Ref. [7].

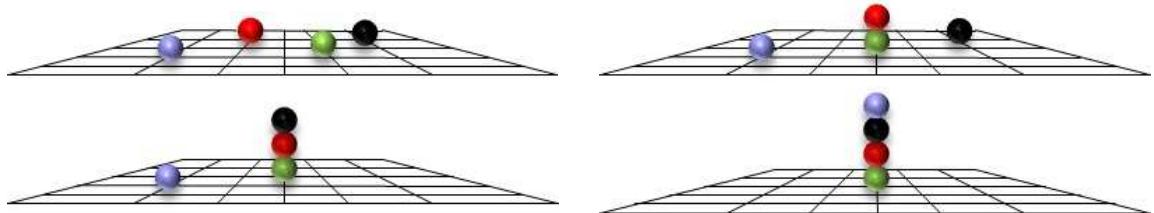
In this talk, I will report on the first ever *ab initio* calculation of the Hoyle state and discuss a new look on the phenomenon of clustering in nuclei, which emerges naturally in the framework of nuclear lattice simulations. This new approach to the nuclear many-body problem is based on the forces derived from the chiral effective Lagrangian of Quantum Chromodynamics (QCD). For few-nucleon systems, the chiral effective field theory (EFT) for the forces between two, three and four nucleons has been worked out up to next-to-next-to-next-to-leading order ( $\text{N}^3\text{LO}$ ) in the chiral power counting for the nuclear potential. This potential consists of long-range pion exchange(s) and shorter ranged multi-nucleon contact interactions. Bound and scattering states

<sup>1</sup> An *ab initio* calculation is defined as follows: First, one determines the parameters that appear in the nuclear force entirely from a fit to observables in systems with  $A \leq 4$ . Then, the so-determined forces are used without modification in an exact solution of the  $A$ -body problem,  $A \geq 5$ .

are calculated based on exact solutions of the Lippmann-Schwinger or Faddeev-Yakubowsky equations. This method has passed many tests as reviewed in Ref. [8]. To tackle systems with more than four nucleons, a novel scheme that combines these forces with Monte Carlo methods that are so successfully used in lattice QCD was recently developed. This novel scheme is termed “nuclear lattice simulations”. For its foundations and early applications, see the review by Lee [9].

## 2. The framework of nuclear lattice simulations

Here, I very briefly review the framework of nuclear lattice simulations. For more details, I refer e.g. to Refs. [10, 11, 12, 13]. To be able to evaluate the generating functional  $Z_A = \langle \psi_A | \exp(-tH) | \psi_A \rangle$  by numerical methods, space-time is discretized in Euclidean time  $t$  on a torus of volume  $L_s \times L_s \times L_s \times L_t$ , with  $L_s(L_t)$  the side length in spatial (temporal) direction.  $H$  is the nuclear Hamiltonian derived from the chiral effective Lagrangian of QCD and  $\psi_A$  is a Slater determinant for  $Z$  protons and  $N$  neutrons, with  $Z + N = A$ . The minimal distance on the lattice, the so-called lattice spacing, is  $a$  ( $a_t$ ) in space (time). This entails a maximum momentum on the lattice,  $p_{\max} = \pi/a$ , which serves as an UV regulator of the theory. A typical lattice spacing used in the actual simulations is  $a \simeq 2$  fm, corresponding to a momentum cut-off of about 300 MeV. In contrast to lattice QCD, the continuum limit  $a \rightarrow 0$  is not taken. The nucleons are point-like particles residing on the lattice sites, whereas the nuclear interactions (pion exchanges and contact terms) are represented as insertions on the nucleon world lines using standard auxiliary field representations. For the further discussions, it is important to realize which configurations to put nucleons on the lattice are possible. These are displayed in Fig. 1. Of particular importance are the configurations with four fermions on one site in harmony with the Pauli principle. In fact, in a leading order calculation using the two independent four-nucleon contact operators without derivatives  $\sim (\psi^\dagger \psi)^2$ , one finds that in the  ${}^4\text{He}$  system the ground state is severely overbound and consists almost entirely of the quantum state with all four nucleons occupying the same lattice site. This is in part due to a combinatorial enhancement of the contact interactions when more than two nucleons occupy the same lattice site. This effect is partly overcome by higher order four-nucleon operators, but it is most efficiently dealt with by a Gaussian smearing procedure, which turns the point-like vertex into an extended structure. For more details, see Ref. [11]. There is one further issue to be discussed. The nuclear forces have an approximate spin-isospin SU(4) symmetry (Wigner symmetry) [14] that is of fundamental importance in suppressing the malicious sign oscillations that plague any Monte Carlo (MC) simulation of strongly interacting fermion systems at finite density. For this reason, nuclear lattice simulations allow access to a large part of the phase diagram of QCD, whereas calculations using lattice QCD are limited to finite temperatures and small densities (baryon chemical potential).



**Figure 1.** Topologically different configurations to put nucleons on a lattice. From the left upper to the lower right corner: all four nucleons on different sites, two/three/four nucleons on one site, respectively.

	$0_1^+$	$0_2^+$	$2_1^+, J_z = 0$	$2_1^+, J_z = 2$
LO [ $O(Q^0)$ ]	−110(2)	−94(2)	−92(2)	−89(2)
NLO [ $O(Q^2)$ ]	−93(3)	−82(3)	−87(3)	−85(3)
IB + EM [ $O(Q^2)$ ]	−85(3)	−74(3)	−80(3)	−78(3)
NNLO [ $O(Q^3)$ ]	−91(3)	−85(3)	−88(3)	−90(4)
Experiment	−92.16	−84.51	−87.72	

**Table 1.** Lattice results for the ground state  $0_1^+$  and the low-lying excited states of  $^{12}\text{C}$ . For comparison the experimentally observed energies are shown. All energies are in units of MeV.

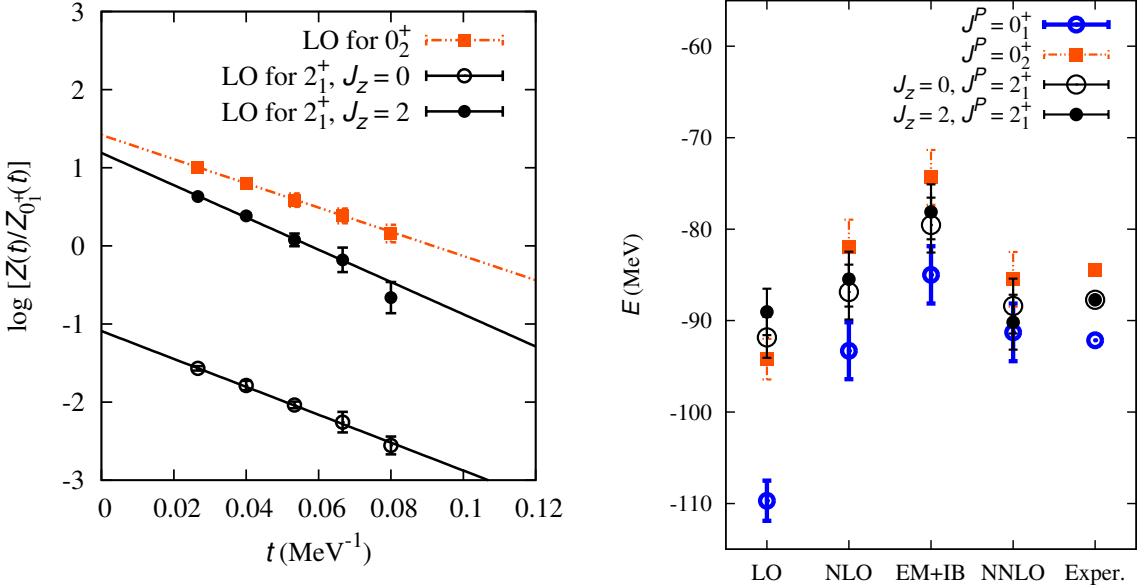
### 3. Ab initio calculation of the carbon-12 spectrum

So far, we have performed calculations at  $\text{N}^2\text{LO}$  in the chiral expansion of the nuclear potential. In the two-nucleon system, we have nine parameters that are determined from a fit to the S- and P-waves in  $np$  scattering. Two further isospin-breaking parameters are determined from the  $pp$  and  $nn$  scattering lengths. The Coulomb force between protons is also included. The three-nucleon force features only two low-energy constants, that can be determined from the triton binding energy and low-energy neutron-deuteron scattering in the doublet channel [13]. The first non-trivial predictions of our approach are the energy dependence of the  $pp$   $^1S_0$  partial wave, which agrees with the Nijmegen partial wave analysis up to momenta of about the pion mass and the binding energy difference between the triton ( $^3\text{H}$ ) and  $^3\text{He}$ . We find  $E(^3\text{H}) - E(^3\text{He}) = 0.78(5)$  MeV, in good agreement with the experimental value of 0.76 MeV [15, 16]. The ground state energies of nuclei with  $A = 4, 6, 12$  were also calculated in these papers.

Our NLEFT collaboration<sup>2</sup> has recently completed *ab initio* lattice calculations of the low-energy spectrum of  $^{12}\text{C}$  using chiral nuclear EFT [17]. In addition to the ground state and the excited spin-2 state<sup>3</sup>, we find a resonance with angular momentum zero and positive parity at  $−85(3)$  MeV, very close to the  $^4\text{He} + ^8\text{Be}$  threshold at  $−86(2)$  MeV. This is nothing but the Hoyle state. To arrive at these results, it was of prime importance to further improve the action as compared to the earlier ground state energy calculations. In particular, the effects of the finite lattice spacing and the unphysical mixing of partial waves due to the breaking of the rotational symmetry was minimized. In addition, we have developed a multi-channel projection Monte Carlo technique that allows to extract excited states from combinations of initial standing waves with zero total momentum and even parity. In Table 1, I show results for ground state and the low-lying excited states of  $^{12}\text{C}$  at leading order (LO), next-to-leading order (NLO), next-to-leading order with isospin-breaking and electromagnetic corrections (IB + EM), and next-to-next-to-leading order (NNLO). For comparison, the experimentally observed energies are also listed. The error bars in Table 1 are one standard deviation estimates which include both Monte Carlo statistical errors and uncertainties due to extrapolation at large Euclidean time. Systematic errors due to the omitted higher-order interactions can be estimated from the size of corrections from  $O(Q^0)$  to  $O(Q^2)$  and from  $O(Q^2)$  to  $O(Q^3)$ . In Fig. 2 (left panel) the lattice results used to extract the excited state energies at leading order are shown. For each excited state we plot the logarithm of the ratio of the projection amplitudes,  $Z(t)/Z_{0_1^+}(t)$ , at leading order.  $Z_{0_1^+}(t)$  is the ground state projection amplitude, and the slope of the logarithmic function at large  $t$  gives the energy difference between the ground state and the excited state.

<sup>2</sup> NLEFT stands for Nuclear Lattice Effective Field Theory.

<sup>3</sup> The orientation bias in our initial state ensemble leads to the splitting of the  $J_z = 0$  and  $J_z = 2$  components of the spin-2 excited state.



**Figure 2.** Left: Extraction of the excited states of  $^{12}\text{C}$  from the time dependence of the projection amplitude at LO. The slope of the logarithm of  $Z(t)/Z_{O_1^+}(t)$  at large  $t$  determines the energy relative to the ground state. Right: Summary of the results for the  $^{12}\text{C}$  spectrum and comparison with experiment. For each order in chiral EFT labeled on the abscissa, results are shown for the ground state (blue circles), the Hoyle state (red squares) and the  $J_z = 0$  (open black circles) and  $J_z = 2$  (filled black circles) projections of the lowest-lying spin-2 state.

Note that within the interval of Euclidean time shown, the results for the excited states are very clean and thus allow for an unambiguous and precise extraction of the corresponding energies. As seen in Tab. 1 and summarized in Fig. 2 (right panel), the NNLO results for the Hoyle state and spin-2 state are in agreement with the experimental values. While the ground state and spin-2 state have been calculated in other studies, these results are the first *ab initio* calculations of the Hoyle state with an energy close to the phenomenologically important  $^8\text{Be}$ -alpha threshold. Experimentally the  $^8\text{Be}$ -alpha threshold is at  $-84.80$  MeV, and the lattice determination at NNLO gives  $-86(2)$  MeV. We also note the energy level crossing involving the Hoyle state and the spin-2 state. The Hoyle state is lower in energy at LO but higher at NLO. One of the main characteristics of the NLO interactions is to increase the repulsion between nucleons at short distances. This has the effect of decreasing the binding strength of the spinless states relative to higher-spin states. We note the 17 MeV reduction in the ground state binding energy and 12 MeV reduction for the Hoyle state while less than half as much binding correction for the spin-2 state. This degree of freedom in the energy spectrum suggests that at least some fine-tuning of parameters is needed to set the Hoyle state energy near the  $^8\text{Be}$ - $^4\text{He}$  threshold. It would be very interesting to understand which fundamental parameters in nature control this fine-tuning. At the most fundamental level there are only a few such parameters, one of the most interesting being the masses of the up and down quarks. Some investigations have already been performed to unravel the quark mass dependence of the deuteron binding energy and of the S-wave nucleon-nucleon scattering lengths [19, 20]. The impact on the primordial abundances of light elements created by a variation of the quark masses at the time of Big Bang nucleosynthesis was also studied in Ref. [21]. Along similar lines, we are presently studying the quark mass dependence of the  $^{12}\text{C}$  spectrum.

#### 4. A new look at clustering in nuclear physics

The cluster model of nuclei, that was initiated by Hstad, Teller and others many decades ago [22], naturally explains the maxima in the binding energy per particle observed for nuclei with even and equal numbers of protons and neutrons. All these nuclei starting with  $^8\text{Be}$  can be considered as composed of alpha-particles. For  $^8\text{Be}$ , the dumbbell-like structure emerging from two close-by alphas could be even demonstrated in the ab initio calculation of Ref. [23]. Alpha-clustering also plays an important role in the Hoyle-state, higher excited states in  $^{12}\text{C}$  and the analogous states in  $^{16}\text{O}$ , as discussed by Martin Freer at this conference [5]. In this classical picture, such states are composed of  $\alpha$ -particles in various geometrical configurations, e.g. the Hoyle state is visualized as three loosely bound alphas in a shallow potential, that leads to weak binding and easy break-up corresponding to  $\alpha$ -radioactivity. In such a picture, the Hoyle state has a much larger charge radius than the ground state, although in more realistic models including configuration mixing allowing for shell-model components one finds some reduction in size [7].

The framework discussed here offers a fresh - and may be very different - look at the phenomenon of clustering. As shown in Fig. 1, configurations with up to four nucleons (two protons and two neutrons with spin up and down, respectively) on one lattice site are possible. Thus,  $\alpha$ -type of clustering is inherent in this approach. As already mentioned above, if one uses leading order interactions with no smearing, one encounters a cluster instability, such that e.g. the ground state of  $^4\text{He}$  is severely overbound and consists almost entirely of the quantum state with all four nucleons occupying the same lattice site. This can be understood as the result of two contributions. First, the LO four-fermion interactions are momentum-independent and thus too strong at high momenta. Second, there is a combinatorial enhancement of the contact interactions when more than two nucleons occupy the same lattice site (for a more detailed discussion, see [11]). This effect is known from studies of two-dimensional large-N droplets with zero-range attraction and also from systems of higher-spin fermions in optical traps and lattices [24, 25, 26]. Within chiral EFT, this problem is cured by either going to higher orders and including the corresponding higher derivative operators or, even better, to perform a Gaussian smearing of the contact interactions with its size tuned to the nucleon-nucleon effective ranges. This improved LO action that acts differently on the S- and P-waves is then used in the nonperturbative part of the calculation while all other higher order operators are treated in perturbation theory. Thus, one effectively has given the LO contact interactions some extension. Furthermore, as a consequence of dealing with this phenomenon, we have essentially given a new meaning to clustering in nuclei - one does not have to think in terms of classical  $\alpha$ -particles but rather in terms of smeared out states with four nucleons on one lattice site. One might contemplate how this new picture in the continuum limit  $a \rightarrow 0$  might recover the old one - such a question can be addressed in the formulation of lattice chiral EFT of Montvay and Urbach [27], who propose to introduce a momentum cut-off independent of taking the continuum limit. Clearly, lots of work is required to solidify the arguments leading to this novel look at clustering, but I am quite confident that the successful calculation of the  $^{12}\text{C}$  spectrum has already offered us a first hint, as explained here.

#### 5. Summary and outlook

Nuclear lattice simulations are a tool to investigate the structure of atomic nuclei based on the forces derived from the chiral Lagrangian of QCD. Besides the the  $^{12}\text{C}$  nucleus and the Hoyle state discussed here, our collaboration has also investigated dilute neutron matter in the unitary limit [28] and is presently addressing the issue of possible P-wave pairing in neutron matter. If existing for physical strength of the P-wave interactions, it would certainly have consequences for the nuclear equation of state and the cooling rate of neutron stars. Nuclear reaction dynamics can also be addressed within this framework, however, more conceptual developments are necessary.

A first step in this direction was recently performed. In Ref. [29] it was shown that bound states moving in a finite periodic volume have an energy correction which is topological in origin and universal in character. The topological volume corrections contain information about the number and mass of the constituents of the bound states. These phase corrections should be considered when determining scattering phase shifts for composite objects at finite volume (this work has been extended to quantum field theory in a finite volume in Ref. [30]). Such investigations pave the way for a model-independent calculation of the unsatisfactorily determined reaction  $^{12}C(\alpha, \gamma)^{16}O$  at stellar energies. This process plays an important role in the element synthesis in stars and in the dynamics underlying supernova explosions. It is often called the “holy grail” of nuclear astrophysics. The framework presented here holds the promise to solve this outstanding problem and thus might contribute significantly to our understanding of the generation of the elements needed for life on Earth.

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